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Free Energy Estimates and Asymptotic Behaviour of Reaction–Diffusion Processes

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Abstract. We prove a class of inequalities closely related to Poincaré's Inequality. Roughly speaking, these inequalities state that for many reaction–diffusion systems the free energy can be estimated by the corresponding dissipation rate. This allows to describe the asymptotic behaviour of such reaction–diffusion systems without using global uniform bounds for the concentrations.

1. Introduction

In this paper we shall deal with reaction–diffusion processes of m species $X_1, \ldots, X_m$, which can be modeled by equations of the following form:

$$\frac{\partial u_i}{\partial t} - \operatorname{div}(d_i \operatorname{grad} u_i) = \sum_{\rho=1}^{r} (k_\rho u^{\alpha_\rho} - k'_\rho u^{\beta_\rho})(\beta_{\rho i} - \alpha_{\rho i}) \text{ in } \Omega, \quad i = 1, \ldots, m, \tag{1}$$

$$\frac{\partial u_i}{\partial \nu} = 0 \text{ on } \partial\Omega, \quad i = 1, \ldots, m. \tag{2}$$

Here $u = (u_1, \ldots, u_m)$ is a vector of concentrations and the right hand side of (1) represents reactions

$$\alpha_{\rho 1} X_1 + \ldots + \alpha_{\rho m} X_m \rightleftarrows \beta_{\rho 1} X_1 + \ldots + \beta_{\rho m} X_m, \quad \rho = 1, \ldots, r,$$

of mass action type. For an explanation of the notation used in (1), (2) see the next section.

Systems of reactions of mass action type have been investigated, e.g., by Horn and Jackson [HJ], Horn [Ho], and Feinberg [Fei]. Starting from their results some years ago we proved in [Gr] (in a somewhat more general context) that a trajectory of a system of type (1), (2) approaches exponentially a spatially homogeneous thermodynamic equilibrium if only this trajectory is globally bounded. The assumption of global boundedness is rather unpleasant. In this paper we shall avoid such an assumption. We shall prove under weak hypotheses that the (suitably scaled) free energy is not only a Lyapunov function for the system (1), (2) but decays exponentially as time tends to infinity.

The main tool for our investigation of asymptotic behaviour is a class of inequalities closely related to Poincaré's Inequality. These inequalities show that, for a large class of reaction diffusion systems, the free energy can be estimated by the corresponding dissipation rate.

In the next section we introduce the necessary notation and recall a result on stationary solutions to (1), (2), which is important for our considerations. Section 3 is devoted to the formulation and the proof of the main results. In the last section we shall indicate possible generalizations and discuss some simple examples.

2. Preliminaries

Throughout this paper Ω denotes a bounded Lipschitzian domain in $\mathbb{R}^N$. With respect to the data of our reaction–diffusion system, i.e., the coefficients of diffusion $d_1, \dots, d_m$, the coefficients of reaction $k_1, \dots, k_r$, $k'_1, \dots, k'_r$, and the vectors of stoichiometric coefficients $\alpha_1, \dots, \alpha_r$, $\beta_1, \dots, \beta_r$ we assume that

$$\left.\begin{aligned} &d_i \in L^\infty(\Omega),\ d_i \geq c_0 > 0, \quad i = 1, \dots, m, \\ &k_\rho \in L^\infty(\Omega),\ k'_\rho \in L^\infty(\Omega),\ k_\rho \geq c_0 > 0,\ k'_\rho \geq c_0 > 0, \quad \rho = 1, \dots, r, \\ &\alpha_\rho \in \mathbb{Z}^m_+,\ \beta_\rho \in \mathbb{Z}^m_+, \quad \rho = 1, \dots, r. \end{aligned}\right\} \tag{A1}$$

As usual, for $u \in \mathbb{R}^m$ and $\alpha \in \mathbb{Z}^m_+$, we define $u^\alpha := u_1^{\alpha_1} \cdot \ldots \cdot u_m^{\alpha_m}$. The elements of $\mathbb{R}^m_+$ will also be regarded as constant functions on Ω. This will not lead to misunderstandings. Moreover, we define $\mathbb{P}^m := \operatorname{int} \mathbb{R}^m_+$.

Essential for our results is the assumption

$$E := \left\{ e \in \mathbb{P}^m : k_\rho e^{\alpha_\rho} = k'_\rho e^{\beta_\rho},\ \rho = 1, \dots, r \right\} \neq \emptyset. \tag{A2}$$

This means that there exists a spatially homogeneous simultaneous equilibrium for all pairs of reactions. In general the set E consists of more than one point (cf. Theorem 1 below). **For the remaining part of this paper we fix** $e \in E$**.** We define

$$F(u) := \int_\Omega \sum_{i=1}^m \int_{e_i}^{u_i(x)} \log \frac{y}{e_i}\, dy\, dx \quad \text{for } u \in L^2(\Omega; \mathbb{R}^m_+). \tag{3}$$

The elements of $L^2(\Omega; \mathbb{R}^m_+)$ will be interpreted as *states* of the system under consideration, and $F(u)$ will be called the *free energy* of the state u. Later we shall discuss the dependence of F on the choice of e (see Remark 3 below).

It is easily checked that the functional F is strictly convex on $L^2(\Omega; \mathbb{R}^m_+)$. Moreover, $F(u) \geq 0$, and $F(u) = 0$ if and only if $u = e$. The Gâteaux derivative $\mu = F'(u)$, if it exists, is the vector of the *chemical potentials* corresponding to the state u. From (3) it follows, at least formally, that $\mu = (\mu_1, \dots, \mu_m) = \log \frac{u}{e}$. Here and later we use the following notation: If $v \in \mathbb{R}^m_+$, $w \in \mathbb{P}^m$ then $\frac{v}{w}$ and $\log w$ mean the vectors with the components $\frac{v_i}{w_i}$ and $\log w_i$, respectively.

Now we shall give a precise meaning to the problem (1), (2).

Let $V := H^1(\Omega; \mathbb{R}^m) \cap L^\infty(\Omega; \mathbb{R}^m))$, let V_+ be the usual positive cone in V, and let V^* be the dual to V. We define $A : V \longrightarrow V^*$ by

$$\langle Au, v \rangle := \int_\Omega \sum_{i=1}^m \left\{ d_i \operatorname{grad} u_i \cdot \operatorname{grad} v_i + \sum_{\rho=1}^r k_\rho e^{\alpha_\rho} \left[\left(\frac{u}{e}\right)^{\alpha_\rho} - \left(\frac{u}{e}\right)^{\beta_\rho} \right] (\alpha_{\rho i} - \beta_{\rho i}) v_i \right\} dx. \tag{4}$$

Then the problem (1), (2) can be written precisely as follows:

$$\frac{du}{dt} + Au = 0, \quad u \in L^2_{loc}(\mathbb{R}_+; H^1(\Omega; \mathbb{R}^m_+)) \cap L^\infty_{loc}(\mathbb{R}_+; L^\infty(\Omega; \mathbb{R}^m)); \tag{I}$$

here $\frac{du}{dt}$ denotes the derivative of u with respect to time in the sense of V^*-valued distributions. The spaces occurring in (I) have the usual meaning (see, e.g., [Zei]). The requirement $u \in L^\infty_{loc}(\mathbb{R}_+; L^\infty(\Omega; \mathbb{R}^m))$ could be replaced by a weaker one, but this is not important for our purposes.

Let u be a solution to (I). Then u is a function of time t with values in V. As is known from thermodynamics, the corresponding dissipation rate is

$$-\frac{d}{dt}F(u(t)) = -\left\langle \frac{du}{dt}(t), \mu(t) \right\rangle$$

Eliminating $\frac{du}{dt}$ by means of (I) we obtain for the dissipation rate:

$$-\frac{d}{dt}F(u(t)) = \int_\Omega \sum_{i=1}^m \Big\{ d_i \operatorname{grad} u_i(t) \cdot \operatorname{grad} \log u_i(t)$$

$$+ \sum_{\rho=1}^r k_\rho e^{\alpha_\rho} \left[\left(\frac{u(t)}{e}\right)^{\alpha_\rho} - \left(\frac{u(t)}{e}\right)^{\beta_\rho} \right] (\alpha_{\rho i} - \beta_{\rho i}) \log \frac{u_i(t)}{e_i} \Big\} dx$$

$$= \int_\Omega \left\{ \sum_{i=1}^m 4d_i |\operatorname{grad} \sqrt{u_i(t)}|^2 + \sum_{\rho=1}^r k_\rho e^{\alpha_\rho} \left[\left(\frac{u(t)}{e}\right)^{\alpha_\rho} - \left(\frac{u(t)}{e}\right)^{\beta_\rho} \right] \log \left(\frac{u(t)}{e}\right)^{\alpha_\rho - \beta_\rho} \right\} dx.$$

Therefore, for all functions $u \in V_+$, we define the *dissipation rate*

$$D(u) := \int_\Omega \left\{ \sum_{i=1}^m 4d_i \, |\operatorname{grad} \sqrt{u_i}|^2 + \sum_{\rho=1}^r k_\rho e^{\alpha_\rho} \left[\left(\frac{u}{e}\right)^{\alpha_\rho} - \left(\frac{u}{e}\right)^{\beta_\rho} \right] \log \left(\frac{u}{e}\right)^{\alpha_\rho - \beta_\rho} \right\} dx. \tag{5}$$

(If $\sqrt{u_i} \notin H^1(\Omega)$ for some $i \in \{1, \ldots, m\}$ or precisely one of the two expressions $(\frac{u}{e})^{\alpha_\rho}$, $(\frac{u}{e})^{\beta_\rho}$ vanishes, then $D(u)$ is to be interpreted as $+\infty$.) We want to find conditions guaranteeing

$$F(u) \le c\, D(u) \text{ for some positive constant } c. \tag{6}$$

If (6) were true for all $u(t)$, where again u denotes a solution to (I), then we would have

$$\frac{d}{dt}F(u(t)) = -D(u(t)) \le -\frac{1}{c}F(u(t)),$$

and $F(u(t))$ would decrease as $\exp(-t/c)$.

Remark 1. Let u be a solution to (I). Then, as is easily checked,

$$\int_\Omega (u(t) - u(0))dx \in \mathcal{S} := \text{span}\,\{\beta_1 - \alpha_1, \ldots, \beta_r - \alpha_r\}\,. \tag{7}$$

The space $\mathcal{S}$ will be called the *stoichiometric subspace* of $\mathbb{R}^m$.

The following theorem gives some information about the stationary solutions to (I), in particular about the set E of equilibria introduced in (A2).

Theorem 1.

i) If $Au = 0$, where $u_i \geq 0$, $u_i \neq 0$, $i = 1, \ldots, m$, then $u \in E$.

ii) $u \in E \Longleftrightarrow \log \frac{u}{e} \in \mathcal{S}^\perp$, $u \in \mathbb{P}^m$. (As usual, $\mathcal{S}^\perp$ denotes the orthogonal complement of $\mathcal{S}$ in $\mathbb{R}^m$.)

iii) For every $a \in \mathbb{P}^m$ the set $(a + \mathcal{S}) \cap E$ consists of a single point.

Remark 2. A result including Theorem 1 has been proved already in [Gr]. For the convenience of the reader we repeat the proof here.

Proof of Theorem 1. i) Let u be a solution to $Au = 0$ such that $u_i \geq 0$, $u_i \neq 0$, $i = 1, \ldots, m$. Let, for the time being, all u_i be larger than a positive ε. Then by means of the test functions $\log(u_i/e_i)$, $i = 1, \ldots, m$, we obtain from $Au = 0$ (cf. the discussion of the dissipation rate above)

$$0 = \int_\Omega \left\{ \sum_{i=1}^m 4d_i \,|\text{grad}\,\sqrt{u_i}|^2 + \sum_{\rho=1}^r k_\rho e^{\alpha_\rho} \left[\left(\frac{u}{e}\right)^{\alpha_\rho} - \left(\frac{u}{e}\right)^{\beta_\rho} \right] \log \left(\frac{u}{e}\right)^{\alpha_\rho - \beta_\rho} \right\} dx. \tag{8}$$

The result (8) remains true also if a positive lower bound for the u_i is not known in advance. This can be shown using the test functions $\log((u_i+\varepsilon)/e_i)$, $i = 1, \ldots, m$, and letting $\varepsilon \longrightarrow 0$. From (8) it follows that the components of u are constant functions. Because of the assumption $u_i \geq 0$, $u_i \neq 0$, $i = 1, \ldots, m$, the components of u must be positive. The relation (8) implies also that

$$\left(\frac{u}{e}\right)^{\alpha_\rho} = \left(\frac{u}{e}\right)^{\beta_\rho}, \quad \rho = 1, \ldots, r. \tag{9}$$

Hence u is in E.

ii) Evidently, $u \in \mathbb{P}^m$ satisfies (9) (and thus belongs to E) if and only if

$$(\alpha_\rho - \beta_\rho) \cdot \log \frac{u}{e} = 0, \quad \rho = 1, \ldots, r, \tag{10}$$

i.e., if and only if $u \in \mathcal{S}^{\perp}$.

iii) Let $a \in \mathbb{P}^m$, and let $M := (a + \mathcal{S}) \cap \mathbb{R}^m_+$. We define

$$f(u) := \sum_{i=1}^{m} \int_{e_i}^{u_i} \log \frac{y}{e_i}\, dy \quad \text{for } u \in \mathbb{R}^m_+.$$

From the properties of f it follows that there exists a unique $u \in M$ where f takes its minimal value on M. For $t > 0$ we have

$$\frac{d}{dt} f\left(u + t(a-u)\right) = \sum_{i=1}^{m} \log \frac{u_i + t(a_i - u_i)}{e_i} (a_i - u_i).$$

This shows that, for sufficiently small $t > 0$, the value $f(u+t(a-u))$ would be strictly less than $f(u)$ if one ore more of the components of u would vanish. By the choice of u this is not possible. Hence all u_i are strictly positive, and

$$0 = \frac{d}{dt} f\left(u + t(\beta_\rho - \alpha_\rho)\right) \Big|_{t=0} = \sum_{i=1}^{m} (\beta_{\rho i} - \alpha_{\rho i}) \log \frac{u_i}{e_i}, \quad \rho = 1, \ldots, r.$$

Consequently (cf. ii)), $u \in (a+\mathcal{S}) \cap E$. Conversely, let $u \in (a+\mathcal{S}) \cap E$. Then, because of ii), the derivatives of f in all directions of $\mathcal{S}$ vanish. Hence u is the unique point of $a + \mathcal{S}$ at which f takes its minimal value.

Remark 3. Let $\overline{e}$ be any point of the set E introduced in (A2), and let $\overline{F}$ be defined in analogy to F by

$$\overline{F}(u) := \int_\Omega \sum_{i=1}^{m} \int_{\overline{e}_i}^{u_i} \log \frac{y}{\overline{e}_i}\, dy\, dx.$$

Then

$$\overline{F}(u) - F(u) := \int_\Omega \sum_{i=1}^{m} \left(u_i \log \frac{e_i}{\overline{e}_i} - e_i + \overline{e}_i \right) dx. \tag{11}$$

According to (10) we have

$$(\beta_\rho - \alpha_\rho) \log \frac{e}{\overline{e}} = 0, \quad \rho = 1, \ldots, r. \tag{12}$$

From (11) and (12) it follows that $\overline{F} - F$ is constant on each of the classes

$$\left\{ u \in L^2(\Omega; \mathbb{R}^m_+) : \int_\Omega u\, dx \in a + \mathcal{S} \right\}, \quad a \in \mathbb{R}^m_+.$$

Remark 4. Using (12) one can easily show that the dissipation rate $D(u)$ defined in (5) is independent of the choice of the equilibrium state e.

3. Main Results

For the formulation of our main results we shall need the following additional assumption:

$$a \in \partial \mathbb{R}^m_+ \cap (e+\mathcal{S}) \Longrightarrow \left(\frac{a}{e}\right)^{\alpha_\rho} \neq \left(\frac{a}{e}\right)^{\beta_\rho} \text{ for some } \rho \in \{1,\dots,r\}. \tag{A3}$$

We know from Theorem 1 that the only equilibrium in $\mathbb{P}^m \cap (e+\mathcal{S})$ is e. Assumption (A3) says that there is no equilibrium in $\mathbb{R}^m_+ \cap (e+\mathcal{S})$ which is on the boundary of $\mathbb{R}^m_+$. Examples of systems satisfying (A3) will be given in the last section. There we shall also discuss the necessity of the assumption (A3) for the validity of our main result.

Finally we assume that

$$p := \max\{|\alpha_1|,\dots,|\alpha_r|,|\beta_1|,\dots,|\beta_r|\} \leq \frac{N}{N-2} \text{ if } N = \dim\Omega > 2. \tag{A4}$$

(As usual, $|\alpha| := \alpha_1 + \dots + \alpha_m$ for every multi-index $\alpha \in \mathbb{Z}^m_+$). The number p is the maximal order of reactions occurring in our system. The assumption (A4) guarantees that u^{α_ρ} and u^{β_ρ} depend continuously in $L^2(\Omega)$ on $u_i \in H^1(\Omega)$, $i = 1,\dots,m$.

Now we are ready to state the main result of the paper.

Theorem 2. *Let the hypotheses* (A1)–(A4) *be satisfied. Then, for every* $R > 0$, *there exists* $c_R > 0$ *such that, for* $u \in V_+$ *satisfying* $F(u) \leq R$, *we have*

$$F(u) \leq c_R \left(D(u) + \left| Q \int_\Omega (u-e)dx \right|^2 \right). \tag{13}$$

Here Q *denotes the projection onto the orthogonal complement of the stoichiometric subspace* $\mathcal{S}$ *of* $\mathbb{R}^m$.

Proof. 1. Suppose that the theorem is false. Then there exist $R > 0$ and sequences (c_n), (u_n) in $\mathbb{R}$ and V_+, respectively, such that $c_n \longrightarrow \infty$ and

$$R \geq F(u_n) = c_n \left(D(u_n) + \left| Q \int_\Omega (u_n - e)dx \right|^2 \right) > 0. \tag{14}$$

In view of the definition of D (cf. (5)) this implies that

$$\lim_{n\to\infty}\int_\Omega |\text{grad}\,\sqrt{u_{ni}}|^2 dx = 0, \quad i = 1,\dots,m. \tag{15}$$

From $F(u_n) \le R$ it follows that the sequence (u_n) is bounded in $L^1(\Omega;\mathbb{R}^m)$. Thus, passing to a subsequence if necessary, we may assume that $(\sqrt{u_{ni}})$ converges in $H^1(\Omega)$ to a constant function which will be written as $\sqrt{a_i}$. Then (14) implies that

$$Q\int_\Omega (a-e)dx = \lim_{n\to\infty} Q\int_\Omega (u_n - e)dx = 0.$$

Thus $a \in e + \mathcal{S}$. We may also assume that $u_{ni}(x) \longrightarrow a_i$ for almost every $x \in \Omega$. Therefore from (14) by means of Fatou's Lemma it follows that

$$\int_\Omega \sum_{\rho=1}^r k_\rho e^{\alpha_\rho}\left[\left(\frac{a}{e}\right)^{\alpha_\rho} - \left(\frac{a}{e}\right)^{\beta_\rho}\right]\log\left(\frac{a}{e}\right)^{\alpha_\rho-\beta_\rho} dx = 0.$$

Consequently,

$$\left(\frac{a}{e}\right)^{\alpha_\rho} = \left(\frac{a}{e}\right)^{\beta_\rho}, \quad \rho = 1,\dots,r.$$

In view of assumption (A3) this is possible only if $a \in \mathbb{P}^m$, and Theorem 1 yields $a = e$. Thus $\sqrt{u_{ni}} \longrightarrow \sqrt{e_i}$ in $H^1(\Omega)$, $i = 1,\dots,m$. This gives $u_n \longrightarrow e$ in $L^q(\Omega;\mathbb{R}^m)$ for some $q > 1$ and $F(u_n) \longrightarrow F(e) = 0$.

2. Let $\lambda_n := \sqrt{F(u_n)}$, and let v_n be defined by $\sqrt{u_{ni}} = \sqrt{e_i}(1 + \lambda_n v_{ni})$, $i = 1,\dots,m$. (Note that $\lambda_n > 0$ by (14).) Then $\lambda_n v_n \longrightarrow 0$ in $H^1(\Omega;\mathbb{R}^m)$. In view of the elementary inequality

$$(\xi-\eta)\log\frac{\xi}{\eta} \ge 4|\sqrt{\xi}-\sqrt{\eta}|^2 \text{ for } \xi,\eta > 0$$

it follows from (14) that

$$1 \ge c_n\int_\Omega \Big\{\sum_{i=1}^m 4d_ie_i|\text{grad}\,v_{ni}|^2$$

$$+\sum_{\rho=1}^r k_\rho e^{\alpha_\rho}\frac{4}{\lambda_n^2}\Big(\prod_{i=1}^m(1+\lambda_n v_{ni})^{\alpha_{\rho i}} - \prod_{i=1}^m(1+\lambda_n v_{ni})^{\beta_{\rho i}}\Big)^2\Big\}dx$$

$$+ c_n\left|Q\int_\Omega\sum_{i=1}^m e_i(\lambda_n v_{ni}^2 + 2v_{ni})dx\right|^2. \tag{16}$$

By definition of λ_n and v_n we have (cf. (3))

$$\lambda_n^2 = \int_\Omega \sum_{i=1}^m e_i \left(2(1+\lambda_n v_{ni})^2 \log(1+\lambda_n v_{ni}) - \lambda_n^2 v_{ni}^2 - 2\lambda_n v_{ni}\right) dx. \tag{17}$$

For every $\varepsilon \in]0,1]$ there exists $c > 0$ such that, for $\xi > -1$,

$$2(1+\xi)^2 \log(1+\xi) - \xi^2 - 2\xi = (2+4\xi+2\xi^2)\log(1+\xi) - \xi^2 - 2\xi$$

$$\leq \begin{cases} 3\xi^2 + 2\xi^3 \leq (3+2c)\xi^2 & \text{for } \xi \leq c \\ 3\xi^2 + 2\xi^{2+\varepsilon} & \text{for } \xi > c \end{cases}.$$

Therefore, (17) implies that, for some positive constant c,

$$1 \leq c \int_\Omega \sum_{i=1}^m (v_{ni}^2 + \lambda_n^\varepsilon |v_{ni}|^{2+\varepsilon}) dx.$$

Since grad $v_{ni} \longrightarrow 0$ in $L^2(\Omega; \mathbb{R}^N)$ (cf. (16)) this is possible only if

$$\inf_{n \in \mathbb{N}} \|v_n\|^2_{H^1(\Omega;\mathbb{R}^m)} > 0. \tag{18}$$

Without loss of generality we may assume that

$$b := \lim_{n\to\infty} \frac{v_n}{\|v_n\|_{H^1(\Omega;\mathbb{R}^m)}}$$

exists in $H^1(\Omega; \mathbb{R}^m)$. Obviously, b does not vanish and is constant on Ω. We are going to show that this leads to a contradiction.

The term in the second line of (16) can be written as follows:

$$4 \sum_{\rho=1}^r k_\rho e^{\alpha_\rho} \Big[\Big(\sum_{i=1}^m (\alpha_{\rho i} - \beta_{\rho i}) v_{ni} \Big)^2 + w_{n\rho} \Big],$$

where $w_{n\rho}$ is a finite sum of terms of the form $\lambda_n^{|\gamma|-2} v_n^\gamma$, $\gamma \in \mathbb{Z}_+^m$, $2p \geq |\gamma| > 2$ (cf. hypothesis (A4)). We remark that

$$\|v_n\|^{-2}_{H^1(\Omega;\mathbb{R}^m)} \int_\Omega \lambda_n^{|\gamma|-2} |v_n^\gamma| dx \leq c \|\lambda_n v_n\|^{|\gamma|-2}_{L^{|\gamma|}(\Omega;\mathbb{R}^m)} \longrightarrow 0.$$

Therefore, dividing (16) by $4c_n \|v_n\|^2_{H^1(\Omega;\mathbb{R}^m)}$ and letting $n \longrightarrow \infty$ we obtain

$$0 \geq \int_\Omega \sum_{\rho=1}^r k_\rho e^{\alpha_\rho} \left(\sum_{i=1}^m (\alpha_{\rho i} - \beta_{\rho i}) b_i \right)^2 dx.$$

Hence

$$\sum_{i=1}^{m}(\alpha_{\rho i}-\beta_{\rho i})b_i=0,\quad \rho=1,\dots,r,$$

i.e., $b\in\mathcal{S}^{\perp}$. Let z_n be the vector the components of which are

$$z_{ni}=\frac{1}{\|v_n\|_{H^1(\Omega;\mathbb{R}^m)}}\int_\Omega e_i(\lambda_n v_{ni}^2+2v_{ni})dx.$$

By (16) $Qz_n\longrightarrow 0$ as $n\longrightarrow\infty$ (cf. (18)). Therefore the limit $z:=\lim_{n\to\infty}z_n$ (which exists) is in $\mathcal{S}$. It has the components $z_i=2e_ib_i|\Omega|$, $i=1,\dots,m$. Here and later on $|\Omega|$ denotes the measure of Ω. Because $b\in\mathcal{S}^{\perp}$ we find

$$0=\sum_{i=1}^{m}b_iz_i=|\Omega|\sum_{i=1}^{m}e_ib_i^2,$$

in contradiction to $b\neq 0$. This contradiction completes the proof of Theorem 2.

Remark 5. An inspection of the preceding proof shows that the assertion of Theorem 2 can slightly be improved. The inequality (13) remains true if the dissipation rate $D(u)$ in that inequality is replaced by the generally smaller term

$$\int_\Omega\left\{\sum_{i=1}^{m}4d_i\,|\mathrm{grad}\,\sqrt{u_i}|^2+\sum_{\rho=1}^{r}4k_\rho e^{\alpha_\rho}\left|\left(\frac{u}{e}\right)^{\alpha_\rho/2}-\left(\frac{u}{e}\right)^{\beta_\rho/2}\right|^2\right\}dx.$$

To see this one has to check the derivation of the inequality (16).

Corollary. *Let the hypotheses of Theorem 2 be satisfied and let u be a solution to* (I). *Moreover, let e be the unique element of E in $\frac{1}{|\Omega|}\int_\Omega u(0)\,dx+\mathcal{S}$ (cf. Theorem 1,iii)). Then, for some $\lambda>0$,*

$$\forall t\geq 0:\quad F(u(t))\leq F(u(0))\exp(-\lambda t).$$

Proof. For $t>0$ and every $\varepsilon>0$ we have

$$F(u(t)+\varepsilon)-F(u(0)+\varepsilon)=\int_0^t\left\langle\frac{du}{dt}(s),\log\frac{u(s)+\varepsilon}{e}\right\rangle ds.$$

Using the equation for $\frac{du}{dt}$ and letting $\varepsilon\longrightarrow 0$ we find

$$F(u(t))+\int_0^t D(u(s))ds\leq F(u(0)).$$

Similarly, for every $\lambda > 0$,

$$\exp(\lambda t)F(u(t)) + \int_0^t \exp(\lambda s)[-\lambda F(u(s)) + D(u(s))]ds \leq F(u(0)).$$

Since $F(u(t)) \leq F(u(0))$ we are in a position to use Theorem 2. Note that

$$Q\int_\Omega (u(s) - e)dx = 0$$

because

$$\int_\Omega (u(s) - e)dx = \int_\Omega (u(s) - u(0) + u(0) - e)dx \in \mathcal{S}$$

(cf. Remark 1 and the condition imposed on e in the formulation of the corollary). Hence Theorem 2 shows that $\lambda F(u(s)) \leq D(u(s))$ and therefore

$$\exp(\lambda t)F(u(t)) \leq F(u(0))$$

for each sufficiently small $\lambda > 0$.

Remark 6. Let

$$d(u, v) := F(u) + F(v) - 2F\left(\frac{u+v}{2}\right) \text{ for arbitrary } u, v \in L^2(\Omega; \mathbb{R}^m_+).$$

Since F is strictly convex we have $d(u, v) \geq 0$, and $d(u, v) = 0$ if and only if $u = v$. As a consequence of (11) the function d is independent of the choice of the equilibrium state e. It is easy to check that, for some positive constants c_δ and C_δ,

$$c_\delta \|u - v\|^2_{L^2(\Omega;\mathbb{R}^m)} \leq d(u, v) \leq C_\delta \|u - v\|^2_{L^2(\Omega;\mathbb{R}^m)}$$

provided that

$$0 < \delta \leq u \leq 1/\delta, \quad \delta \leq v \leq 1/\delta.$$

Hence $d(u, v)$ behaves similar as a square of a distance of u and v. Functions of this type have been used by [GG] and [Ga1, Ga2] for the proof of uniqueness and regularity results.
In view of $F(e) = 0$ and $F \geq 0$ we have $d(u, e) = F(u) + F(e) - 2F(\frac{u+e}{2}) \leq F(u)$. Hence, under the hypotheses of the corollary,

$$d(u(t), e) \leq F(u(t)) \leq F(u(0))\exp(-\lambda t) \text{ for some } \lambda > 0.$$

4. Generalizations and examples

In the following remarks we want to indicate that the result of Theorem 2 can be generalized in several directions.

Remark 7. Theorem 2 and its corollary remain true if the hypothesis with respect to the constants of reaction (cf. (A1)) is replaced by the weaker hypothesis

$$k_\rho \geq 0,\ k'_\rho \geq 0, \quad \int_\Omega k_\rho dx > 0,\ \int_\Omega k'_\rho dx > 0, \quad \rho = 1, \ldots, r.$$

The proof is essentially the same. In particular, we can treat systems, where chemical reactions take place only in a part of the domain Ω.

Remark 8. The definition (4) of the operator A can be generalized as follows:

$$\langle Au, v\rangle := \int_\Omega \sum_{i=1}^{m} \left\{ d_i \operatorname{grad} u_i \cdot \operatorname{grad} v_i + \sum_{\rho=1}^{r} k_\rho e^{\alpha_\rho} \left[\left(\frac{u}{e}\right)^{\alpha_\rho} - \left(\frac{u}{e}\right)^{\beta_\rho} \right] (\alpha_{\rho i} - \beta_{\rho i}) v_i \right\} dx$$

$$+ \int_{\partial\Omega} \sum_{i=1}^{m} \sum_{\rho=r+1}^{s} k_\rho e^{\alpha_\rho} \left[\left(\frac{u}{e}\right)^{\alpha_\rho} - \left(\frac{u}{e}\right)^{\beta_\rho} \right] (\alpha_{\rho i} - \beta_{\rho i}) v_i d\sigma.$$

This means that the equations (1) remain unchanged whereas the boundary conditions (2) are to be replaced by

$$d_i \frac{\partial u_i}{\partial \nu} = \sum_{\rho=r+1}^{s} k_\rho e^{\alpha_\rho} \left[\left(\frac{u}{e}\right)^{\alpha_\rho} - \left(\frac{u}{e}\right)^{\beta_\rho} \right] (\beta_{\rho i} - \alpha_{\rho i}) \quad \text{on } \partial\Omega, \quad i = 1, \ldots, m.$$

These boundary conditions model reactions taking place only on the boundary $\partial\Omega$ of the domain Ω. If the order of these additional reactions does not exceed $\frac{N-1}{N-2}$ if $N > 2$ then Theorem 2 is again true. The proof is to be modified in an obvious manner. In the same way one could treat reactions taking place on a part of the boundary or on an interface separating parts of the domain Ω.

Remark 9. It would be desirable to generalize the main inequality proved above to the following cases:

i) The underlying reaction system is no longer reversible but only weakly reversible (see [Fei] or [Gr] for a definition of that notion).

ii) The species can be electrically charged.

iii) The relations between chemical potentials and concentrations are given by $\mu_i = \log(g_i(u)u_i)$, $i = 1, \ldots, m$, where $g_i(u)$ is the so called coefficient of activity of the species X_i, which is a known function of the vector of all concentrations.

In these cases the definitions of $F(u)$ and $D(u)$ have to be modified appropriately.

Example 1. Let two species react as follows:

$$X_1 + X_2 \rightleftarrows 0.$$

This means that the reaction of X_1 and X_2 produces something which is available to such an amount that it is not necessary to include it in the balance equations. The corresponding reaction term is $ku_1u_2 - k' = k(u_1u_2 - K)$. For the sake of simplicity we assume that k, k', and K are positive constants. Then

$$E = \left\{e \in \mathbb{P}^2 : \ e_1e_2 = K\right\}.$$

The assumptions (A1), (A2), (A3), (A4) are satisfied, if $N \leq 4$. It is easy to see that $\mathcal{S}^\perp = \text{span}\,\{(1,-1)\}$ and

$$Q(v_1, v_2) = \frac{1}{2}(v_1 - v_2, v_2 - v_1).$$

Theorem 2 says that

$$\int_\Omega \sum_{i=1}^{2} \int_{e_i}^{u_i} \log \frac{y}{e_i} dy\, dx \leq c_R \left\{ \int_\Omega \Big(\sum_{i=1}^{2} |\text{grad}\, \sqrt{u_i}|^2 + (u_1u_2 - K) \log \frac{u_1u_2}{K} \Big) dx + \left| \int_\Omega (u_1 - e_1 - u_2 + e_2) dx \right|^2 \right\}$$

provided that the left hand side is less or equal R. In particular, for every $e > 0$,

$$\int_\Omega \sum_{i=1}^{2} \int_{e}^{u_i} \log \frac{y}{e} dy\, dx \leq c_R \left\{ \int_\Omega \Big(\sum_{i=1}^{2} |\text{grad}\, \sqrt{u_i}|^2 + (u_1u_2 - e^2) \log \frac{u_1u_2}{e^2} \Big) dx + \left| \int_\Omega (u_1 - u_2) dx \right|^2 \right\}$$

provided that the left hand side is less or equal R.

Example 2. We assume that the reactions $X_i \rightleftarrows 0$, $i = 1, \ldots, m$, take place on the boundary $\partial\Omega$. This corresponds to the boundary conditions

$$d_i \frac{du_i}{\partial \nu} = k_i(e_i - u_i), \ i = 1, \ldots, m, \ \text{ on } \partial\Omega.$$

For the stoichiometric vectors we have

$$\alpha_{ji} = \delta_{ji},\ \beta_j = 0,\ j = 1, \dots, m.$$

Consequently, $\mathcal{S} = \mathbb{R}^m$ and $Q = 0$. Hence the assumptions (A1)–(A4) are satisfied. Theorem 2 gives

$$\int_\Omega \sum_{i=1}^m \int_{e_i}^{u_i} \log \frac{y}{e_i} dy\, dx \le c_R \sum_{i=1}^m \left\{ \int_\Omega |\text{grad}\, \sqrt{u_i}|^2 dx + \int_{\partial\Omega} (u_i - e_i) \log \frac{u_i}{e_i} d\sigma \right\}$$

provided the left hand side is less or equal R.

Example 3. Assume that we are given only one species X and that the reaction $X \rightleftarrows 2X$ takes place in Ω. Let the corresponding reaction term be $u - u^2$. Then $E = \{1\}$ and $\mathcal{S} = \mathbb{R}$. In this example the assumption (A3) is not satisfied: 0 is a stationary solution. The inequality

$$\int_\Omega \int_1^u \log y\, dy\, dx \le c_R \int_\Omega \left(|\text{grad}\, \sqrt{u}|^2 + (u^2 - u) \log u \right) dx$$

fails for every constant c_R for u near 0.

This example is typical: If (A3) is not satisfied then there exists a (spatially homogeneous) state u such that $D(u) = 0$ and $u \in e + \mathcal{S}$ whereas $F(u) > 0$.

Example 4. Let the reactions $X_1 + X_2 \rightleftarrows 2X_3$ take part in Ω, and let the reaction term be $u_1 u_2 - u_3^2$. Then $E = \left\{ e \in \mathbb{P}^3 :\ e_1 e_2 = e_3^2 \right\}$, $\alpha = (1, 1, 0)$, $\beta = (0, 0, 2)$, and $\mathcal{S} = \text{span}\,\{(1, 1, -2)\}$. We choose $e = (1, 1, 1)$. The asssumptions (A1), (A2), (A3), (A4) are satisfied, if $N \le 4$. Theorem 2 gives

$$\int_\Omega \sum_{i=1}^3 \int_1^{u_i} \log y\, dy\, dx \le c_R \left\{ \int_\Omega \left(\sum_{i=1}^3 |\text{grad}\, \sqrt{u_i}|^2 + (u_1 u_2 - u_3^2) \log \frac{u_1 u_2}{u_3^2} \right) dx \right.$$

$$\left. + \left| \int_\Omega (u_1 - u_2) dx \right|^2 + \left| \int_\Omega (u_1 + u_2 + u_3 - 3) dx \right|^2 \right\}$$

provided that the left hand side is less or equal R.

Remark 10. Simple examples show that in general the constant c_R in Theorem 2 cannot be chosen independent of R, i.e. one cannot prove that

$$F(u) \le c \left(D(u) + \left| Q \int_\Omega (u - e) dx \right|^2 \right) \quad \text{for all } u \in V_+.$$

Remark 11. In the introduction we have stressed the fact that for our results on the asymptotic behaviour of reaction–diffusion systems global bounds for the concentrations are not necessary. It seems worth mentioning that for a special reaction–diffusion system Glitzky, Gröger, and Hünlich [GGH] were able to prove the existence of global bounds for the concentrations using the main result of this paper.

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